Overview

Deriving scientific information from large, complex datasets can motivate large, complex statistical models, in fields as diverse as astronomy [Regier et al., 2019], economics [Meager, 2019], phylogenetics [Pritchard et al., 2000], and many more. As models grow in complexity, the need to interrogate their assumptions and to propagate uncertainty among their components grows, as does the computational cost of doing so using traditional statistical methods. Many classical procedures designed to address these concerns, such as Markov Chain Monte Carlo (MCMC), cross validation, or re-estimating a model under a range of modeling assumptions, can be prohibitively expensive in many modern problems.

To address this gap, my work employs *sensitivity analysis*, applied not merely in the traditional sense of assessing the risk of to imprecise modeling assumptions (though I do pursue this traditional role as well), but also to quantify frequentist sampling properties and propagate uncertainty in Bayesian procedures. Though conceptually unified, my work is diverse in applications, touching many of the core activities of modern data analysis, from cross-validation [Giordano et al., 2019b,a], scalable Bayesian posterior inference [Giordano et al., 2018a,b], the bootstrap [Giordano and Broderick, 2020], and more. A recurrent theme of my work is adapting classical *theoretical tools* [Reeds, 1976, Gustafson, 1996] to *modern computing environments* equipped with scalable, general purpose automatic differentiation software [Baydin et al., 2017, Carpenter et al., 2015].

Data sensitivity: cross validation and frequentist variance

Accuracy bounds for approximate cross validation. To perform leave-one-out CV (LOO-CV), one re-runs an estimation procedure with each datapoint left out. In full, LOO-CV requires as many re-runs procedures as there are datapoints, and each re-run is expected to be quite close to the original fit. Rather than re-running exactly, one can use a Taylor series to approximate the effect of removing a single data point; since the dataset with one point left out is, in some sense, "close" to the original dataset, the Taylor series can be expected to perform well.

Prior to our work, this idea had been suggested both in the machine learning literature [Rad and Maleki, 2018, Koh and Liang, 2017] as well as in the classical statistical literature under the name "infinitesimal jackknife" [Jaeckel, 1972, Shao and Tu, 2012]. However, the machine learning work developed independently of the statistical precedent, and both treatments required unrealistic theoretical conditions for the accuracy of the Taylor series: specifically, that the gradients of the objective function be uniformly bounded, a condition that is rarely satisfied in scientific practice, even in the simplest possible example of using maximum likelihood to estimate the sample mean of a normal distribution.

In Giordano et al. [2019b], we synthesized the classical statistics and machine learning developments, providing a more realistic set complexity condition under which the Taylor series is accurate, eschewing the need for bounded gradients. Unlike previous work, our theory was purely finite sample, implying

the asymptotic results of prior work as a corollary. We demonstrated the accuracy of the technique on an unsupervised clustering problem from genomics [Shoemaker et al., 2015].

Sensitivity to removal of a small fraction of the data. Classical frequentist standard errors estimate the variability in an estimator that would result from the rarefied thought experiment of re-sampling datasets from the same distribution that gave rise to the observed data. In the social sciences, this rarefied experiment rarely closely corresponds to reality, and one might be concerned if substantive conclusions could be overturned by other minor perturbations to the data.

In Giordano et al. [2020], we provide an easily-computed approximation to quantify the effect of ablating a small proportion of a dataset, with open-source software and finite-sample accuracy bounds for ordinary least squares and instrumental variables regression. We find that problems with small signal-to-noise ratio but large datasets will be particularly non-robust to the removal of a small proportion of the data. Such a situation that obtains commonly in econometrics, and we find that the sign and statistical significance of estimated effects in a number of large, prominent econometric studies can be overturned by dropping only a small number of datapoints [Angelucci and De Giorgi, 2009, Finkelstein et al., 2012, Meager, 2019].

Frequentist variability of Bayesian posteriors. Bayesian statistics provides powerful tools for coherently treating uncertainty in complex problems, though, when the model is misspecified, the estimated posterior uncertainty may not be meaningful. In principle, however, one might always compute the frequentist sampling variability of a Bayesian posterior quantity, and such a quantity always remains meaningful, even if conceptually distinct from a posterior uncertainty [Waddell et al., 2002, Kleijn and van der Vaart, 2006]. However, standard tools for evaluating frequentist uncertainty, such as the bootstrap [Huggins and Miller, 2019], are extremely computationally intensive, as they typically require re-running an MCMC procedure hundreds of times.

By combining the frequentist IJ [Jaeckel, 1972, Shao and Tu, 2012, Giordano et al., 2019b] approach to frequentist variance with the MCMC-based measures of sensitivity [Gustafson, 2000, Giordano et al., 2018a], we derive the Bayesian infinitesimal jackknife (IJ), which can be used to compute the frequentist variability of Bayesian posterior means without bootstrapping or computing a maximum a-posteriori (MAP) estimate. In a work in progress [Giordano and Broderick, 2020], we extend the Bayesian central limit theorem of Lehmann and Casella [2006], Kass et al. [1990] to prove the consistency of the Bayesian IJ and show its accuracy as an approximation to the bootstrap for a larger number of examples, effectively allowing estimation of frequentist covariances orders of magnitude faster than the bootstrap. We demonstrate the accuracy of our method on datasets from election modeling [Gelman and Heidemanns, 2020], ecology [Kéry and Schaub, 2011], and most of the models from [Gelman and Hill, 2006, Stan

Team, 2017].

Sensitivity for Bayesian analysis

Propagation of uncertainty in scalable Bayesian inference One popular technique to scale Bayesian inference to massive problems is mean field variational Bayes (MFVB) [Wainwright and Jordan, 2008, Blei et al., 2017, Regier et al., 2019]. However, MFVB provides notoriously innacurate posterior uncertainty estimates, even in situations when it estimates the posterior means accurately. In [Giordano et al., 2018a], we develop a method to recover accurate posterior uncertainties from MFVB approximations without needing to fit a more complex model or run MCMC. Computing the LRVB covariance requires solving a linear system, which in scientific applications is often sparse and can be solved using iterative techniques such as conjugate gradient [Nocedal and Wright, 2006, Chapter 5]. We compare LRVB covariances to MCMC on a large number of real-world datasets, including logistic regression on an internet advertising dataset [Criteo Labs, 2014], the Cormack-Jolly-Seber model from ecology [Kéry and Schaub, 2011], and hierarchical generalized linear models from the social sciences [Gelman and Hill, 2006], demonstrating accurate posterior covariances computed over an order of magnitude faster than MCMC.

Hyperparameter sensitivity for MCMC. MCMC is arguably the most commonly used computational tool to estimate Bayesian posteriors, and modern black-box MCMC tools such as `Stan` [Stan Development Team, 2020, Carpenter et al., 2017]. However, MCMC still often takes a long time to run, and systematically exploring alternative prior parameterizations by re-running MCMC would be computationally prohibitive for all but the simplest models. A classical result from Bayesian robustness states that the sensitivity of a posterior expectation is given by a particular posterior covariance [Gustafson, 1996, Basu et al., 1996], though the result has not been widely used, arguably due in part to the lack of an automatic implementation. In my software package, Giordano [2020], I take advantage of the automatic differentiation capacities of `Stan` to provide automatic hyperparameter sensitivity for generic Stan models. In examples in the package `git` repository, I demonstrate the efficacy of the package in detecting excess prior sensitivity, particularly in a social sciences model taken from Gelman and Hill [2006, Chapter 13.5].

Bayesian nonparametrics. A commonly question in unsupervised clustering is how many distinct clusters are present in a dataset. Discrete Bayesian nonparametrics (BNP) allows the answer to be inferred using Bayesian inference, but one must specify a prior on how distinct clusters are generated [Ghosh and Ramamoorthi, 2003, Gershman and Blei, 2012]. A particularly common modeling choice is the stick-breaking representation of a Dirichlet process prior [Sethuraman, 1994], a mathematical abstraction which is arguably better justified by its computational convenience than its realism. Our workshop paper, Giordano

et al. [2018b], fits a BNP model with variational Bayes [Blei and Jordan, 2006] using the standard, computationally convenient stick-breaking prior, but then uses sensitivity analysis to allow the user to explore alternative functional forms an order of magnitude faster than would be possible with refitting. In work currently in progress, we apply our method to a human genome dataset in phylogenetics taken from [Huang et al., 2011], and find that our method accurately discovers real excess prior sensitivity in a BNP version of the model `fastSTRUCTURE` [Raj et al., 2014].

Selected Future work

My research is driven by the needs of my scientific collaborators, and so my future work will be determined to a large part by my colleagues. Here, I will discuss a few directions that I find promising and interesting, and which I believe could be applicable to a diverse set of problems.

Bootstrapping and bootstrapping after bootstrapping. We extend the ideas of Giordano and Broderick [2020] to higher-order Taylor series approximations in Giordano et al. [2019a], provding a family of estimators which we collectively call the higher-order infintiesimal jackknife (HOIJ). In addition to providing higher-quality approximations to CV and extending our results to k-fold CV, the higher-order approach promises to provide a scalable alternative to the bootstrap, a procedure that estimates frequentist variability by repeatedly re-evaluating a model at datasets drawn with replacement from the observed data. The bootstrap is known to enjoy higher-order accuracy in certain circumstances Hall [2013], and the HOIJ can approach the bootstrap at a rate faster than the bootstrap approaches the truth. The HOIJ thus promises to make bootstrap inference available to models which are differentiable but too expensive to re-evaluate (e.g. simulation-based models [Gourieroux and Monfort, 1993]), but also to allow efficient bootstrap-after-bootstrap procedures which that are currently out of reach for all but the simplest statsitics Efron and Tibshirani [1994].

Preprocessing Sensitivity. Analyses in genomics often begin with a preprocessing step in observation units are clustered together according to ad-hoc measures of similarity across a large number of feature vectors [Xu and Su, 2015, Stuart et al., 2019]. Quickly assessing the sensitivity of these procedures to the inclusion or exclusion of individual features would allow the researcher to identify high-leverage observations and avoid imposing structure via arbitrary modeling assumptions. Sensitivity anlaysis cannot be applied directly to such similarity measures, as they are typically non-differentiable. With a colleague from biology, we are investigating using a probabilisitic relaxation only of the initial distance measure, drawing random datasets, and applying the non-differential similarity measure to these random datasets, taking the average similarity across draws as the output of the procedure. We can then assess the sensitivity of the

original sample's probability to inclusion or exclusion of particular features, and assess in turn the sensitivity of the importance sampling estimate of the average output, providing a sensitivity analysis of the whole non-differentiable procedure. Conceptually, approach is attractive because it would allow sensitivity analysis to be applied to black-box procedures without having to design and validate custom continuous relaxations.

Partitioned Bayesian inference. The ideas of [Giordano et al., 2018a] can be naturally extended to approximately propagate uncertainty amongst separately estimated components of an inference problem. For example, astronomical catalogues are customarily produced with MFVB-like algorithms [Lang et al., 2016, Regier et al., 2019], which take inputs such as the sky background and optical point spread function as fixed inputs, though these quantities are themselves inferred with uncertainty. Viewing all the separate inference procedures as a sequential quasi-MFVB objective, one could directly apply the techniques of LRVB to propagate the uncertainty from the modeling inputs to the astronomical catalogue's uncertainty. Doing so would require the approximate solution of a very large, but very sparse, linear system, which is itself an interesting computational challenge.

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